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Ab Initio Equation of State for β-HMX[1] FRANK ZERILLI, Naval Surface Warfare Center, Indian Head, MD, MAIJA KUKLJA, National Science Foundation, Arlington, VA — An ab initio equation of state for the molecular crystal β-octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (β-HMX) has been calculated for temperatures between 0 and 400 K, and for specific volumes from 0.42 to 0.55 cm^3/gm, corresponding to relative volumes from 0.8 to 1.03. The calculated 300 K isotherm agrees well with the experimentally measured pressure-volume relation reported by Gump and Peiris (*J. Appl. Phys.* **97**, 053513 (2005)), and by Yoo and Cynn (*J. Chem. Phys.* **111**, 10229 (1999)). The calculated specific heat agrees well with experimental data reported over the range from 300 to 400 K (Hanson-Parr and Parr, *J. Energetic Mater.* **17**, 1-47 (1999)). The main source of error in the calculations is due to the absence of an adequate ab inito treatment of non local van der Waals interactions which are important in molecular crystals. Work is underway to include these interactions.

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